Effects of Vacancy on Mechanical Properties of Single-Crystal γ-TiAl based on Molecular Dynamics Simulation

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Keywords: γ-TiAl alloy, Molecular dynamics, Vacancy, Crack, Mechanical properties

Abstract. To investigate the effect of vacancy concentrations on mechanical properties of single crystal γ-TiAl, the uniaxial tension tests of γ-TiAl alloy models at different vacancy based on molecular dynamics simulation was performed. The results shows that obvious brittle behavior in stress-strain curve and ultimate stress decreases nonlinearly with increasing vacancy concentrations can be got. When the atom near vacancy is changed, potential energy reaches to maximum, and decreases with the increasing of vacancy concentrations. In the process of tension tests, vacancy gradually is evolved to the hole, and then the hole is evolved to micro cracks. Finally the micro crack extended until the material fractures. The form of crack propagation is different at different vacancy concentrations.

Introduction

In recent years, light and high temperature structure materials are focused on by research. TiAl alloy, as one of the new type structure materials, due to its low density, high conductivity, high specific strength and stiffness, and good capability of flame retardant and oxidation resistant, becomes the material which has huge development potential and application prospect of high temperature. It is widely used in aerospace and automotive. At present, the main applications in TiAl alloy are the engine with high-pressure turbine blade, low pressure turbine, excessive tube beam, exhaust valve, nozzle etc [1-8]. However, the application of TiAl alloy is limited by its damage and defects. In order to make full use of its excellent properties, and make it better used in aerospace, it is necessary to understand its characteristics. Point defect is widespread in crystal materials and is the basic structure of crystal materials. The distribution of point defect in crystal materials is random and disorder. Point defect has huge effect on mechanical properties of materials. Vacancy is one of the point defects, which appears on the location of atoms and only have a size of one atom. So, it is difficult to observe directly by experiment. Using molecular dynamics method to study on metal materials has more advantage than experiment. It can be used to simulate and analyze point defect directly, researchers are attracted by its simple modeling and accurate simulation results [9].

The displacement cascades of neutron irradiation with various vacancy concentrations in bcc-Fe is simulated by Wang [10], the results shows that the defect annihilation is faster in the case of the higher pre-vacancy concentrations. The mechanical properties of single-crystal bulk Mg_2Si is investigated by Yu [11], and the results shows that the ultimate stress decreases nonlinearly with increasing vacancy concentrations. Once such defects are present, there will be a substantial drop of the ultimate stress, and higher concentrations cause further decreases. Effects of vacancy defects on tensile mechanical properties of single graphene sheets are investigated by Han [12], the results shows that the new defects are likely to appearing near one or two atom vacancy defects, and there is a reduction in the tensile strength and failure strain. Because of the exising of vacancy, the effects of temperature and vacancies on crack in graphene sheet are investigated by Lohrasebi[13], the results shows that the presence of vacancy reduces the critical load giving different crack propagation

trajectory. Generation and evolution of vacancy-type defects in nano-Cu films during plastics deformation are investigated by Xu[14] , the results shows that the plastic deformation appears near free surface due to the dislocation nucleation, both the generation and evolution of vacancy-type are related to dislocation activities.

For the past few years, the research of γ-TiAl alloy at atomic scale is still very limited, the research of γ-TiAl alloy using molecular dynamics simulation method are as follows: the shear deformation[15], the tension deformation [16], phase transformation [17], void growth [18], fracture behaviors of <110> tilt grain boundaries [19], Super dislocation of asymmetric nucleation and movement [20].

Aiming at the shortcomings of the above research on γ-TiAl alloy, this work is analyzed for the effect of the vacancy concentrations on mechanical behavior of γ-TiAl alloy, and γ-TiAl alloy models which have vacancy concentrations of 0%, 0.008%, 0.012%, 0.016% and 0.03% are estabilished.

Computational Model and Method

The crystal structure of γ-TiAl is $L1_0$ (face centered square) crystal structure model [21]. Lattice constants are a=4.001 Å, b= 4.001 Å, c= 4.181 Å[18]， the crystal structure is showed as Fig.1.

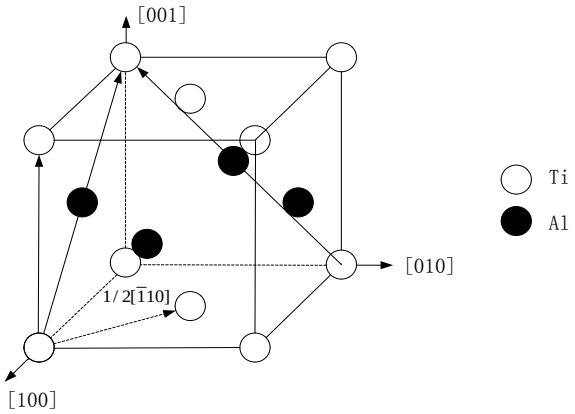

Fig. 1 $L1_0$ structure of γ-TiAl

Embedded atom method potential(EAM)[22] is used in molecular dynamics. The x, y, and z coordinate axes correspond to the crystallographic orientations [100], [010], and [001]. Periodic boundary condition is used in the y direction, and x, z directions with free boundary condition. During the simulation of tensile test, the under surface of model is fixed, and tensile along z axis. In order to convenient tensile, set three layers atom fixed to prevent upper and lower layer atom from the substrate. The temperature is set to 1K to aviod the influence of the heating effect on vacancy, and time step is set to 1fs. Strain rate is set to 1.0×1081/s, which is relatively high, much greater than that used in real experiments. Since the time scale of MD is set by the atomic motion, only a short period of time can be simulated. Thus, realization of a reasonable deformation in such a very short time requires a relatively high strain rate. The simulation is carried out with canonical NVT ensemble, because velocity-verlet algorithm is more accurate than other algorithm. So the algorithm is used in this work to solve the trajectory of atom. LAMMPS, which is an open source software, is used to simulate the tensile test. The Open Visualization Tool (OVITO) is used to demonstrate and analyze atomistic simulation configurations during deformation. OVITO uses the centrosymmetry parameter to highlight defective atoms, and view the evolution of the defects during the shape-change and fracture processes.

The model have 24442 atoms, the potential energy curve and stress-strain curve at different vacancy concentrations(0%, 0.008%, 0.012%, 0.016% and 0.03%)is obtained during the tension test. With the analysis of potential energy, elastic modulus and the ultimate stress, the better understanding for the mechanical properties of γ-TiAl alloy in atom scale can be got.

Results and Discussion

In the process of uniaxial tension, through the analysis for potential energy curve, atomic trajectory, and stress-strain curve at different vacancy concentrations, the effect of vacancy on atomic motion, potential energy and stress is investigated.

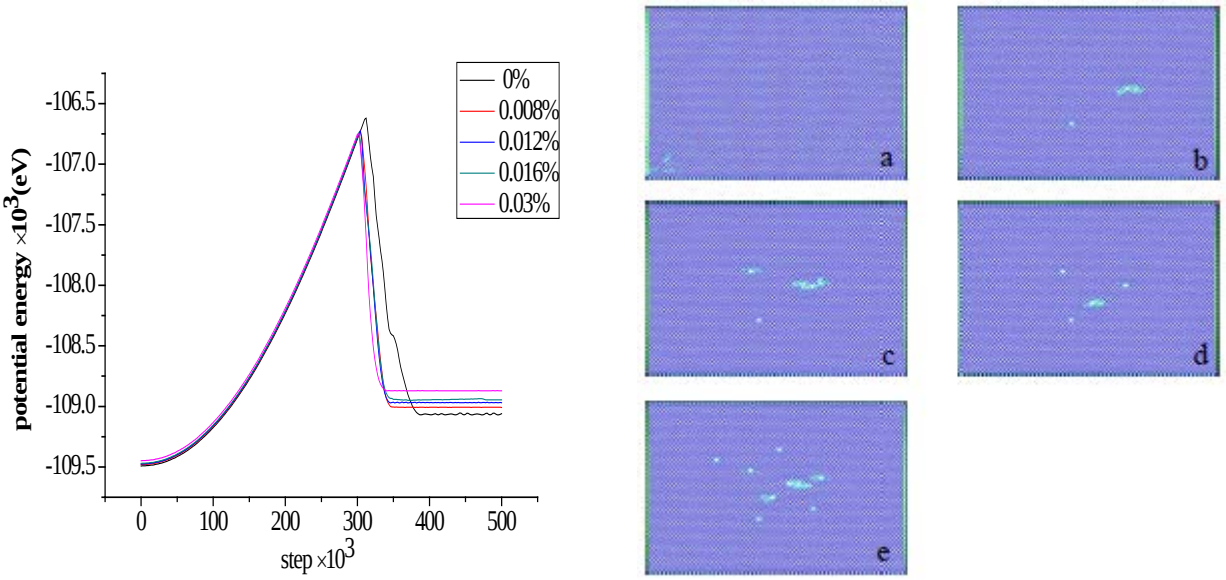

Fig.2 Potential energy as function of the loading time at different vacancy concentrations of γ-TiAl

The change of potential energy for γ-TiAl is showed in Fig. 2. The five atomic trajectories in Fig. 2 (a-e) correspond to the atomic trajectory of ultimate potential energy. What can be got from Fig. 2 is that potential energy curve overlap at initial stage, and shows a trend of increasing. Furthermore, the energy concentrates to the maximum. The distortion appears in the district of vacancy and atom disorder. There is a crack initiation around the vacancy with the increase of time step. Finally, the crack is converged and extended to fracture. During the process, the potential energy declines. The potential energy is balanced when the material fractures. The ultimate potential energy decreases with the increase number of vacancies.

The trajectories of five models are showed in Fig. 3 to Fig.7. Because the thickness is only three layers atoms, it is not convenience to observe the evolution of vacancies. So, a layer of atoms is cut out to observe and analyze.

The initial state of the atom is showed in Fig. 3(a) .The red represents Ti atom, and the blue is Al atom. The rest of the atom trajectory is showed in the center of symmetry parameters of OVITO, which the defects clearly such as dislocation can see easily seen. It can be seen that the Fig. 3 is the tension test simulation which has no vacancy. Due to the influence of boundary, there is dislocation appearing at one corner of the boundary. With the increasing of time step, dislocation move along the slip system. Finally dislocations accumulate at the boundary which leads to stress concentration, and crack easily initates at there. The crack initiation at right boundary propagation alongs the direction of [100], and the crack which initiation at left boundary propagation alongs the direction of $[\bar{1}00]$, finally these two crack converge and propagate until the material fracture.

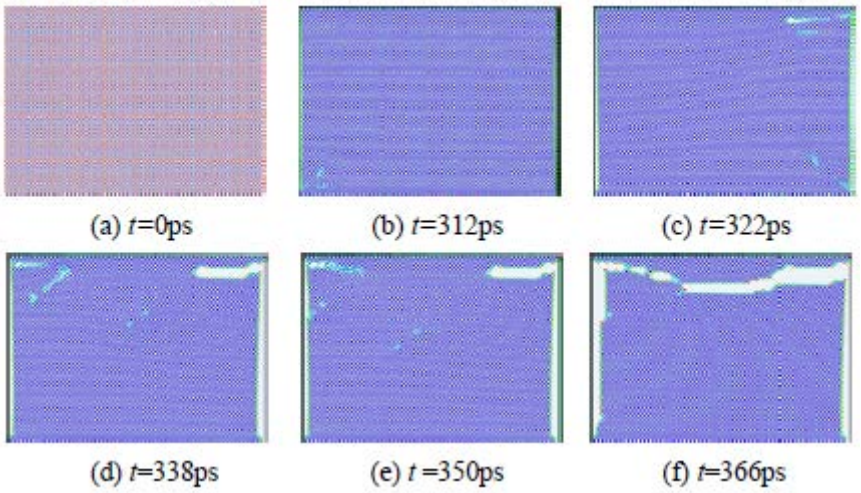

Fig.3 Atomic trajectory at different time with no vacancy

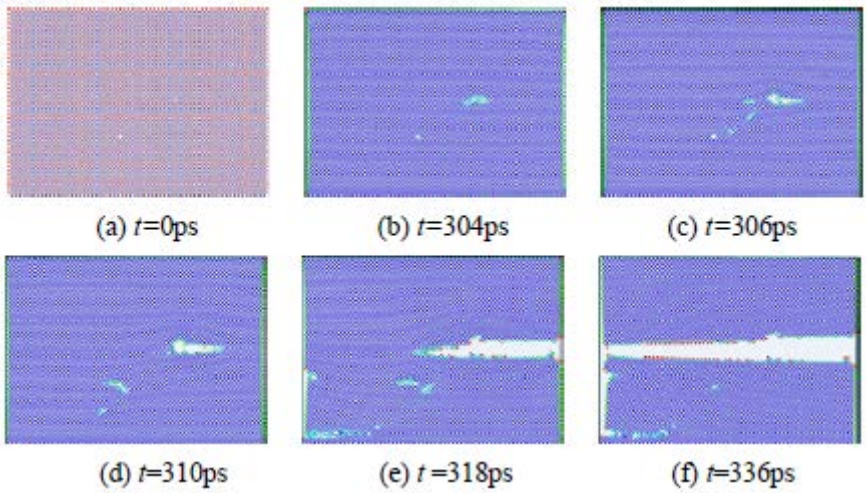

Fig.4 Atomic trajectory at different time with two vacancies

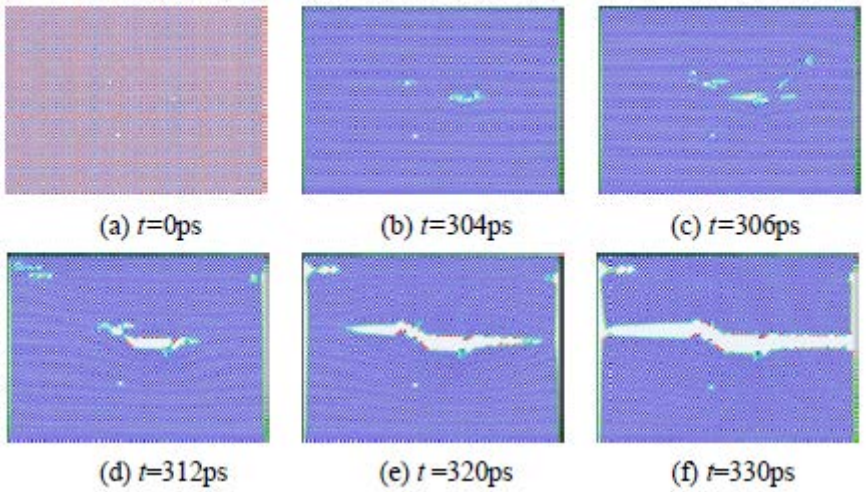

Fig.5 Atomic trajectory at different time with three vacancies

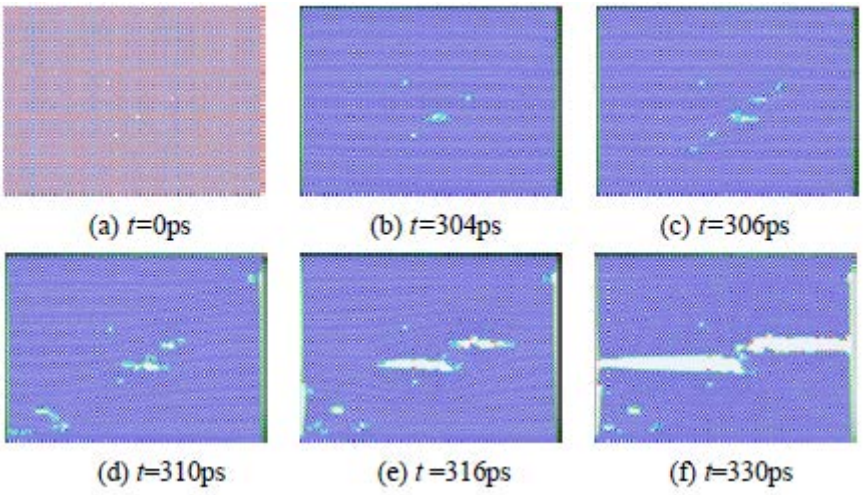

Fig.6 Atomic trajectory at different time with four vacancies

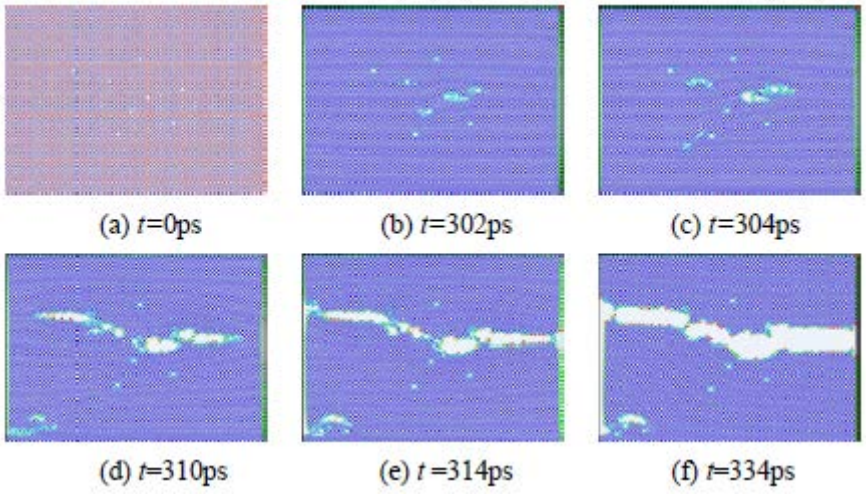

Fig.7 Atomic trajectory at different time with eight vacancies

From Fig.4 to Fig.7, shows that atom becomes disorder easily and this will lead to lattice deformation near the center of the model. As the influence between vacancies, the vacancy which near this vacancy also is changed but others are not. Crack produces at the place which stress concentrate around vacancy as well, crack propagates in different way at different vacancy concentrations.

In order to study the mechanical properties of single crystal γ-TiAl, stress-strain curve are obtained at five models. For each single curve, it can be clearly observed that the stress increases nonlinearly with increasing strain. However, the slope of the curve gradually decreases until failure. Finally, the stress shows a sudden drop at the limit strain, demonstrating typical brittle behavior. Before the stress reaches the maximum, five curves coincide can be seen. Namely, there is no change in the elastic modulus of materials, at the time of atoms disordered and lattice deformation surrounds vacancy. At the same time, stress concentrate to the maximum and relax after the process of vacancy evolves to hole and hole evolves to micro crack. So, the stress declined.

The different vacancy concentrations of limit stress values are showed in Figure 9. It can be seen from the picture that ultimate stress decreases nonlinearly with increasing vacancy concentrations. When the vacancy concentrations are respectively 0%, 0.008%, 0.012%, 0.016% and 0.03%, the corresponding stress values are: 16.12GPa, 15.89GPa, 15.88GPa, 15.85GPa and 15.83GPa. The stress decrease 2% when the vacancy concentrations in γ-TiAl alloy from 0% to 0.03%. Based on the analysis, the vacancy concentration has influence on the ultimate stress.

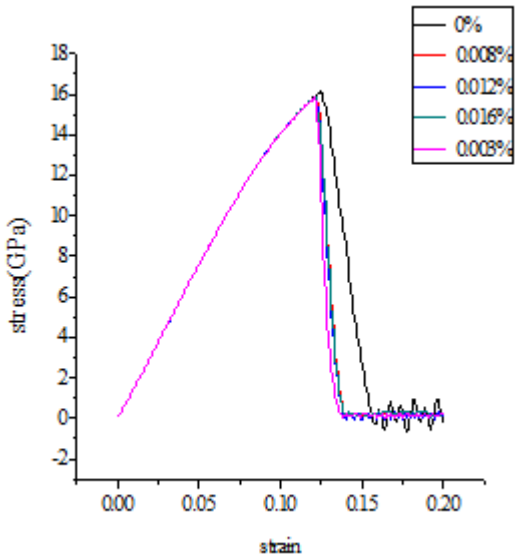

Fig.8 Stress-strain curves at different vacancy concentrations

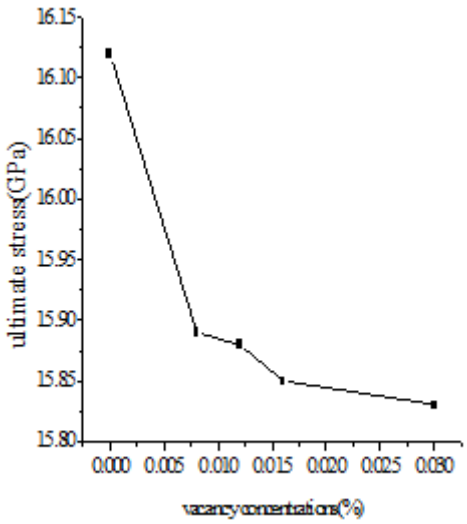

Fig.9 Ultimate stress at different vacancy concentrations

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Conclusion

Molecular dynamics method is applied to the research on mechanical properties of γ-TiAl alloy at different vacancy concentrations. The stress-strain curve of γ-TiAl alloy with vacancy defects shows obvious brittle behavior. Due to the elastic modulus remains constant, the presence of vacancies affects the tensile strength of the material, and ultimate stress decreases nonlinearly with increasing vacancy concentrations. When the vacancy concentrations are low, the limit stress value decreases sharply; when the vacancy concentrations are increased, the limit stress value decreases slowly. At different vacancy concentrations, the form of crack propagation is different.

Acknowledgement

This work was financially supported by National Natural Science Foundation of China(No. 51065014), National Natural Science Foundation of Gansu Province, China (No.148RJZA008), Research project of Gansu Province, China (No.2014A-033). Hai-Yan LI would like to thank Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology for providing help.

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